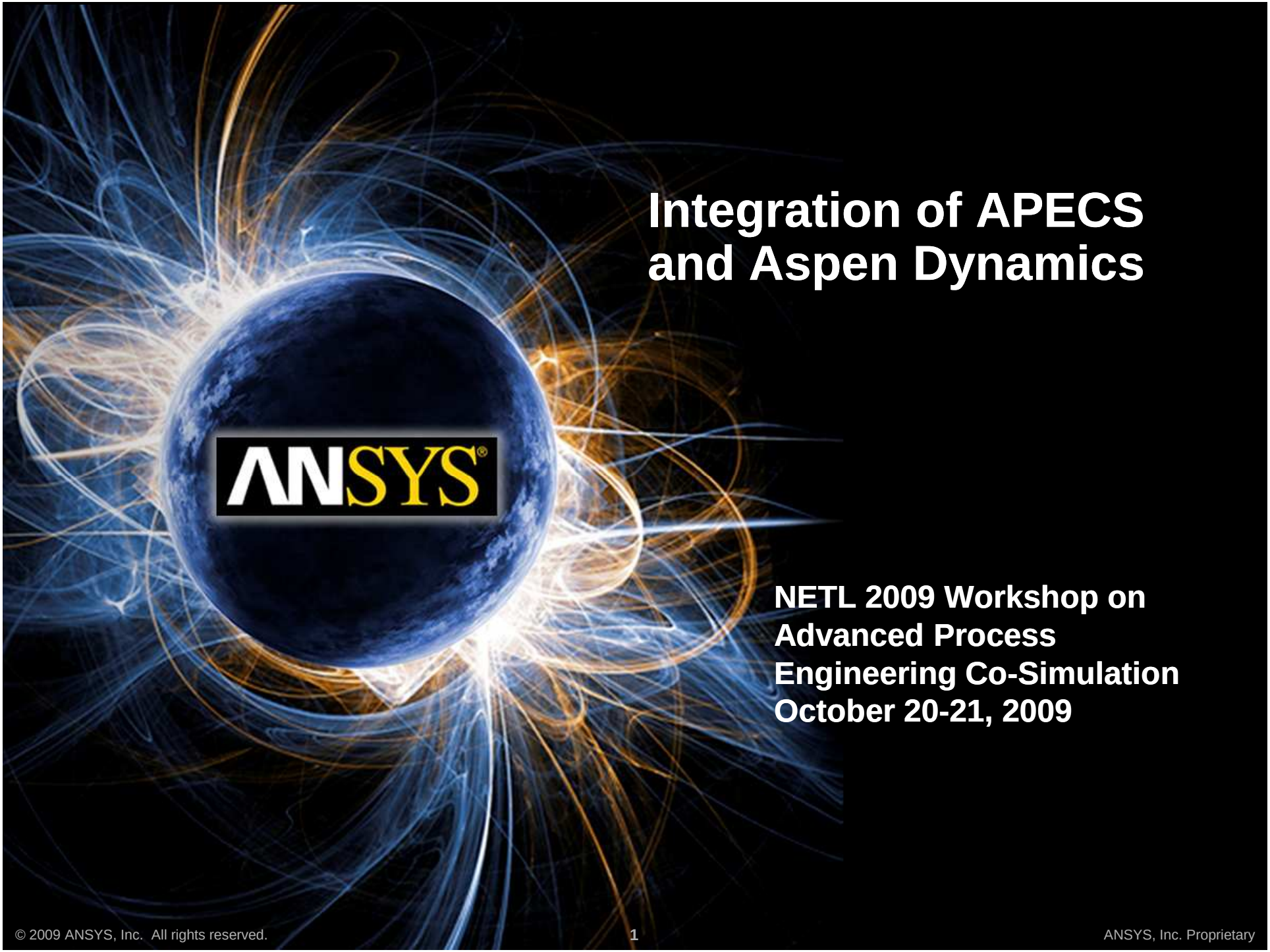

Integration of APECS and Aspen Dynamics

NETL 2009 Workshop on Advanced Process Engineering Co-Simulation
October 20-21, 2009

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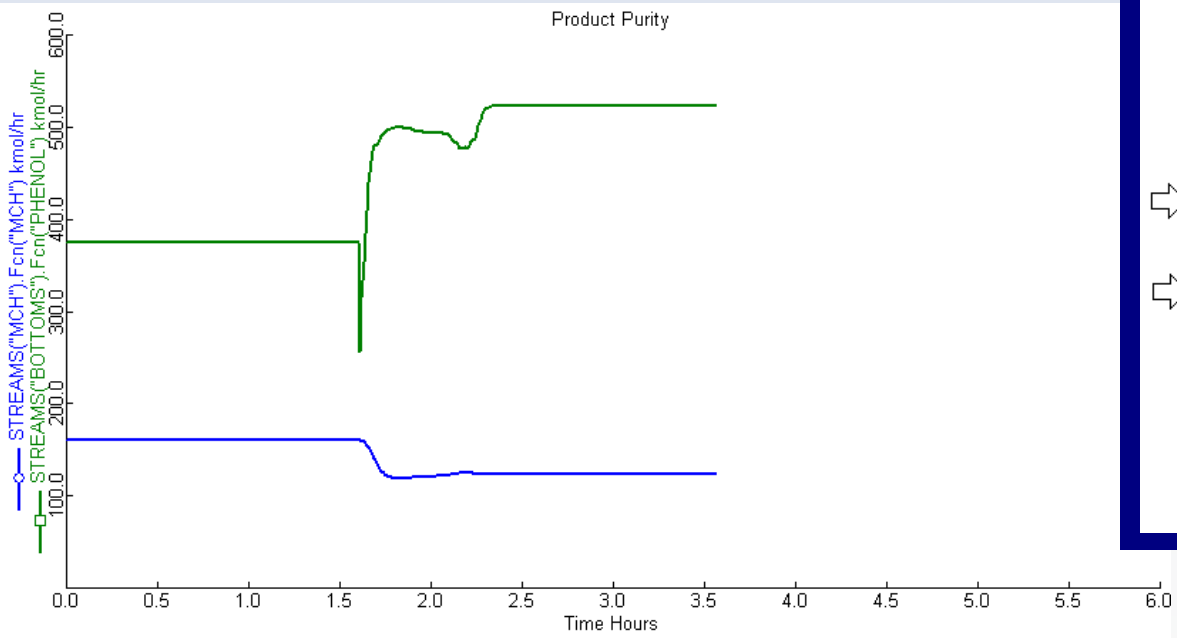
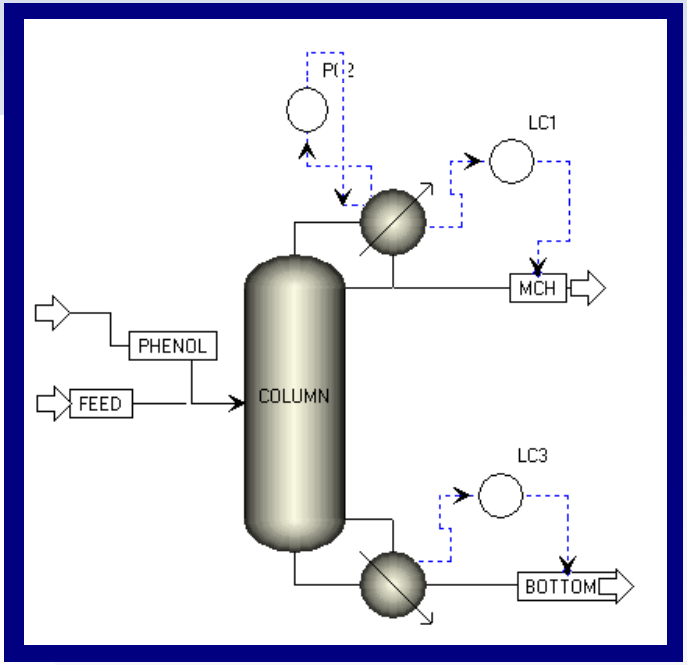
Objective

- **Develop a prototype APECS controller for transient co-simulation**
- **Demonstrate coupling between FLUENT and Aspen Dynamics**





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Technical Issues

- **Aspen Dynamics does not have a CAPE-OPEN block like Aspen Plus**
- **To date, transient simulations have not been considered within the framework of CAPE-OPEN**
- **Unsteady CFD simulations are considerably more time-consuming than steady simulations**
- **Using unsteady CFD simulations within a co-simulation environment poses additional technical difficulties (e.g., "remembering" the initial state)**
  - Assume quasi-steady
  - $\tau_{CFD} << \tau_{Plant}$

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Available Capabilities

- **Aspen Custom Modeler (ACM) permits user-defined blocks to be created and exported**
  - Permits customization at the “block” level
  - Custom blocks can be used in Aspen Dynamics
  - Custom blocks can call external functions
- **Simulation Access eXtension (SAX) capability**
  - Operates at the “flowsheet” level
  - Can call functions at beginning/end of timestep
- **ACM “Events”**
  - Event triggers: OnDeletedBlock, OnNewBlock, etc.
- **ACM Custom Forms**
  - Customized GUI

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Capabilities Used for Prototype

- **Aspen Custom Modeler (ACM) permits user-defined blocks to be created and exported**
  - Permits customization at the “block” level
  - Custom blocks can be used in Aspen Plus Dynamics
  - Custom blocks can call external functions
- **Simulation Access eXtension (SAX) capability**
  - Operates at the “flowsheet” level
  - Can call functions at beginning/end of timestep
- **ACM “Events”**
  - Event triggers: OnDeletedBlock, OnNewBlock, etc.
- **ACM Custom Forms**
  - Customized GUI

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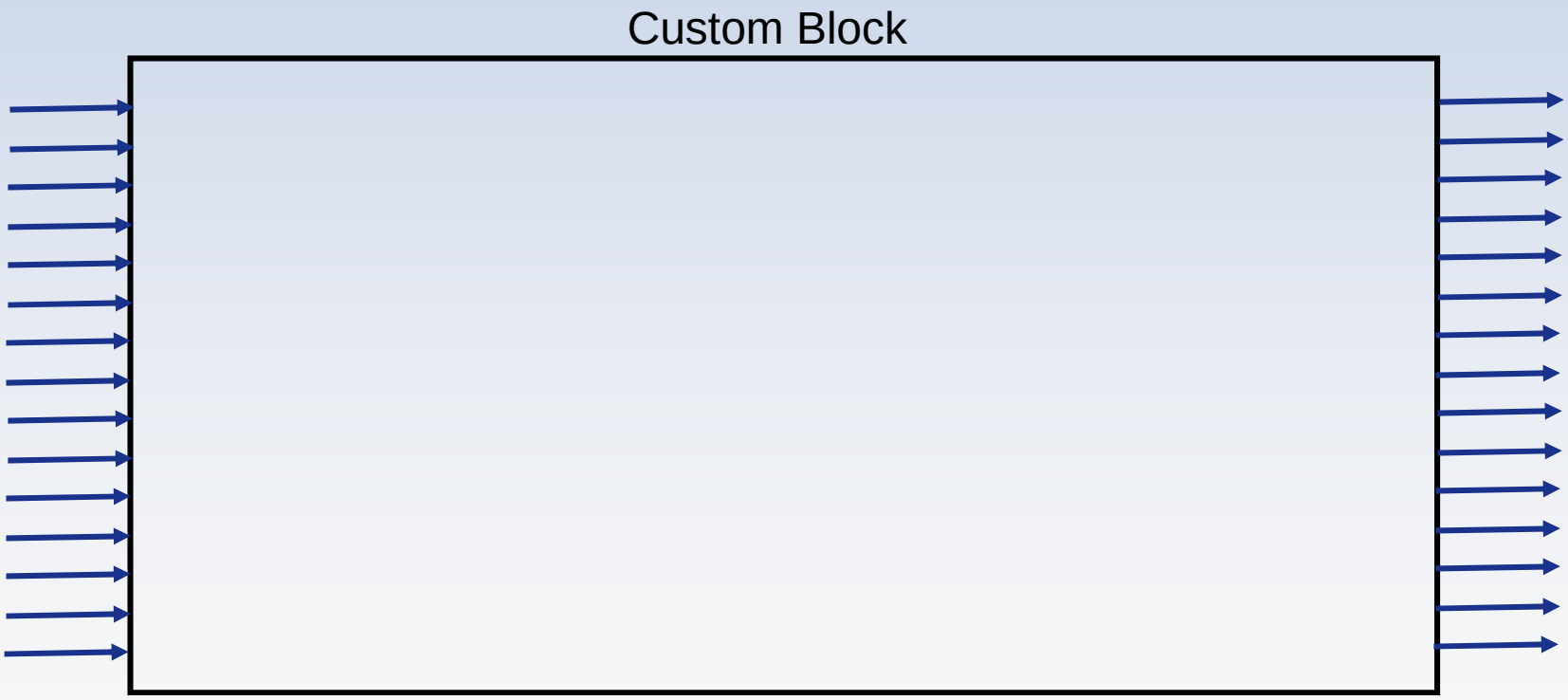
Aspen Dynamics Wrapper

- **Custom block created in Aspen Custom Modeler**



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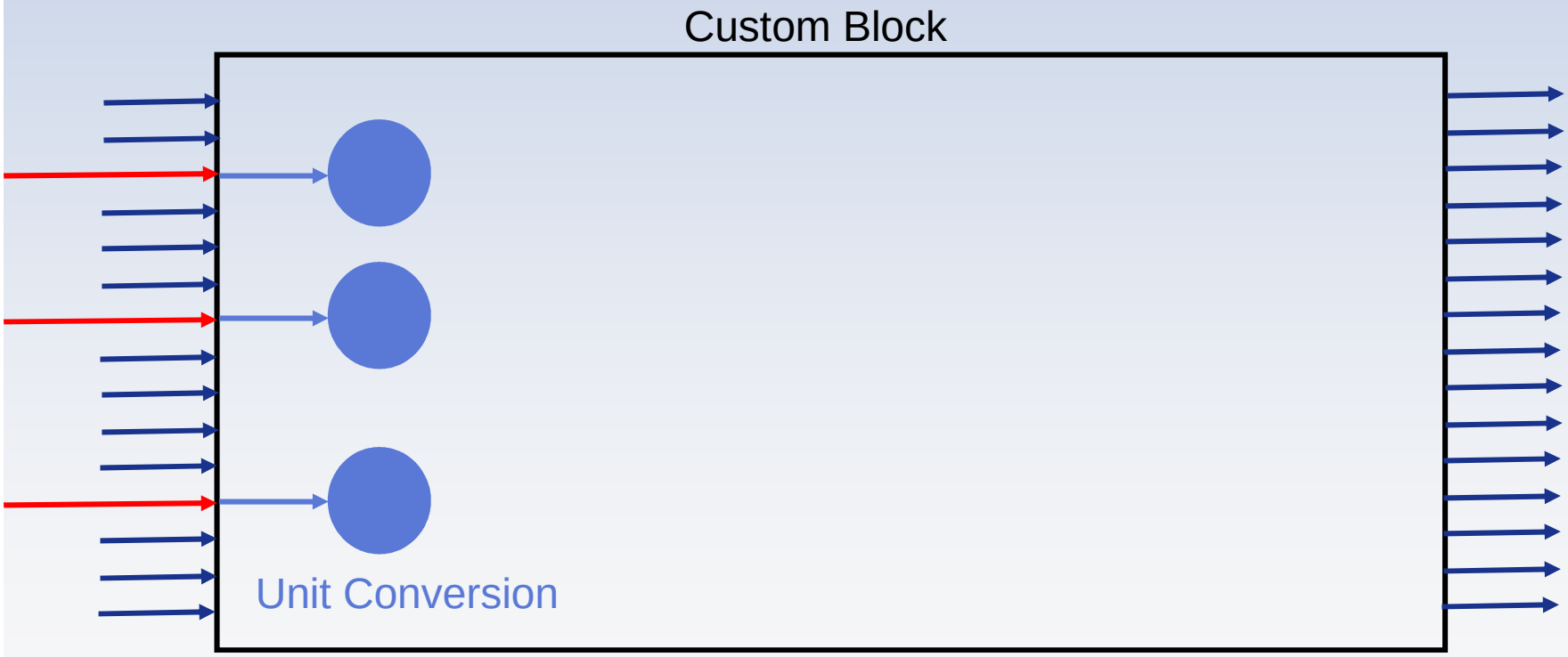
Aspen Dynamics Wrapper (cont.)

- **Custom block created in Aspen Custom Modeler**



Connected Inlet Ports

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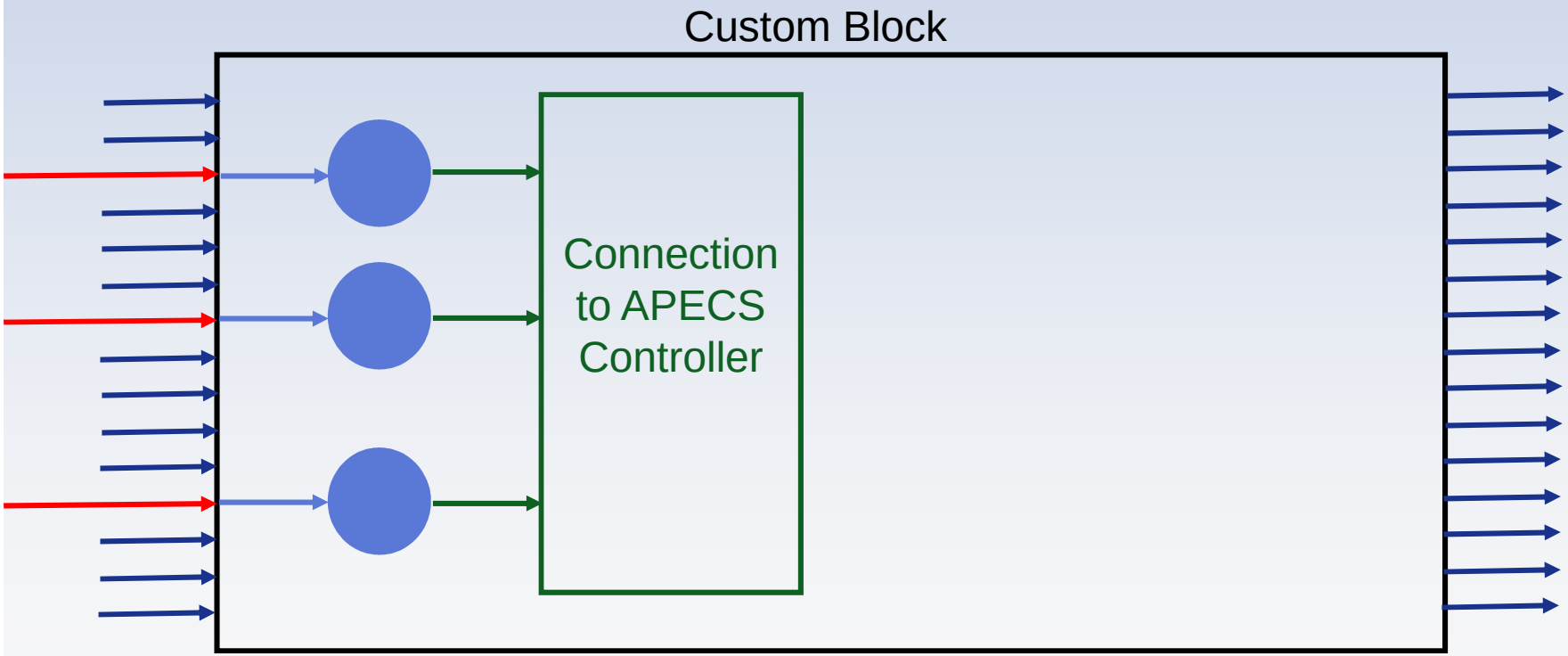
Aspen Dynamics Wrapper (cont.)

- **Custom block created in Aspen Custom Modeler**



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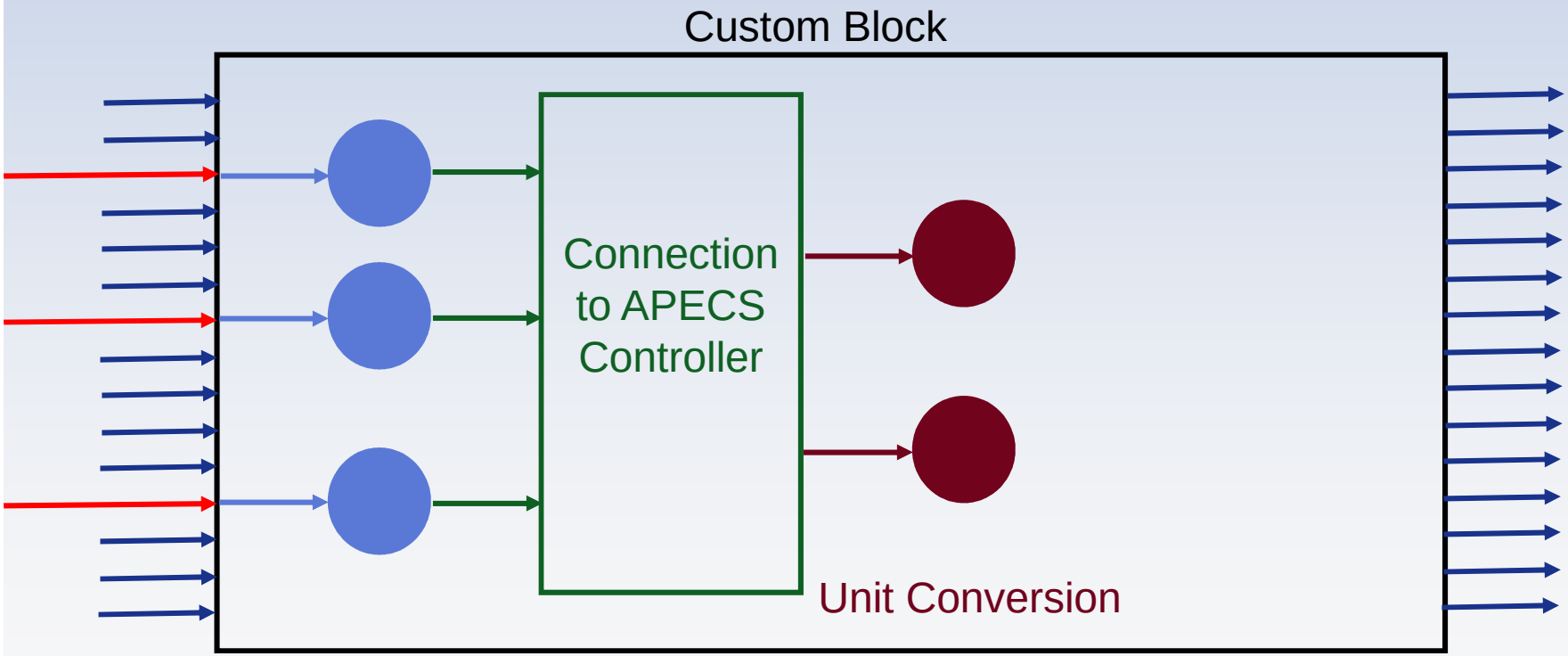
Aspen Dynamics Wrapper (cont.)

- **Custom block created in Aspen Custom Modeler**



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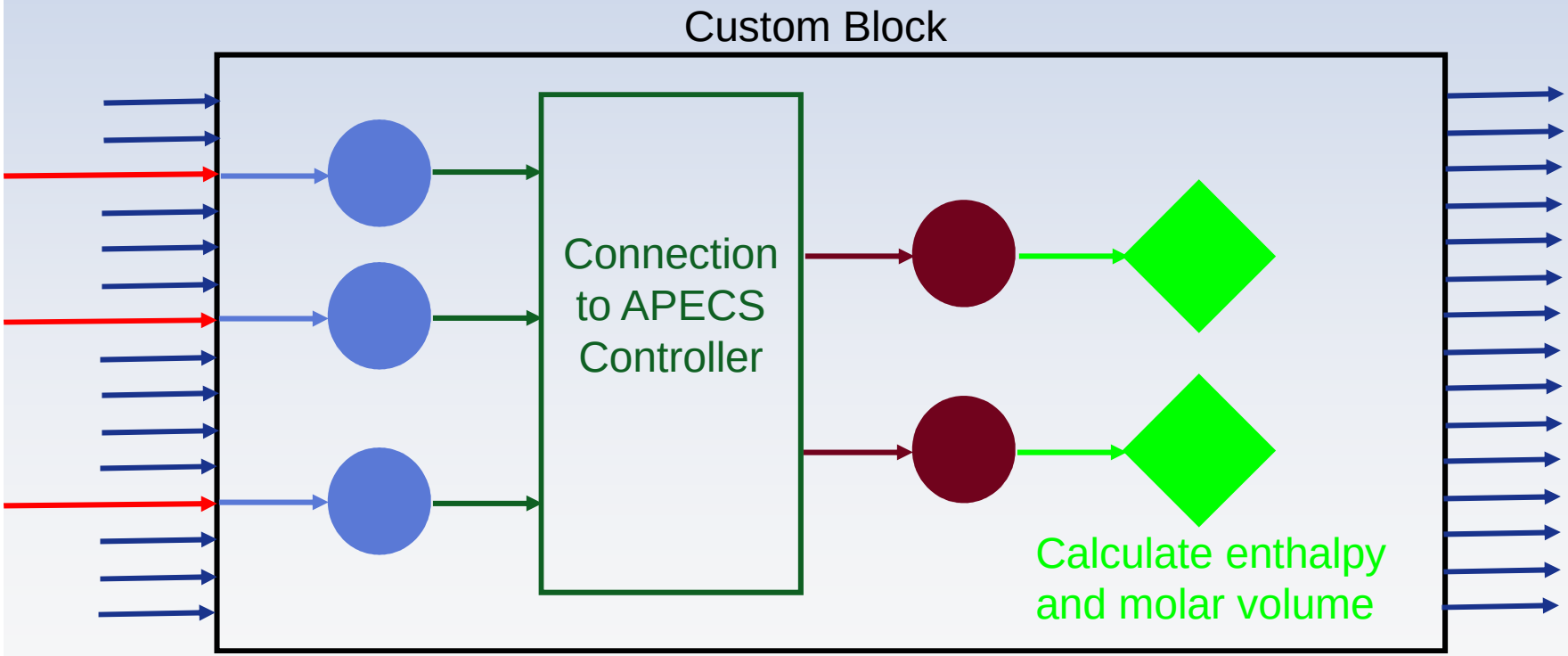
Aspen Dynamics Wrapper (cont.)

- **Custom block created in Aspen Custom Modeler**



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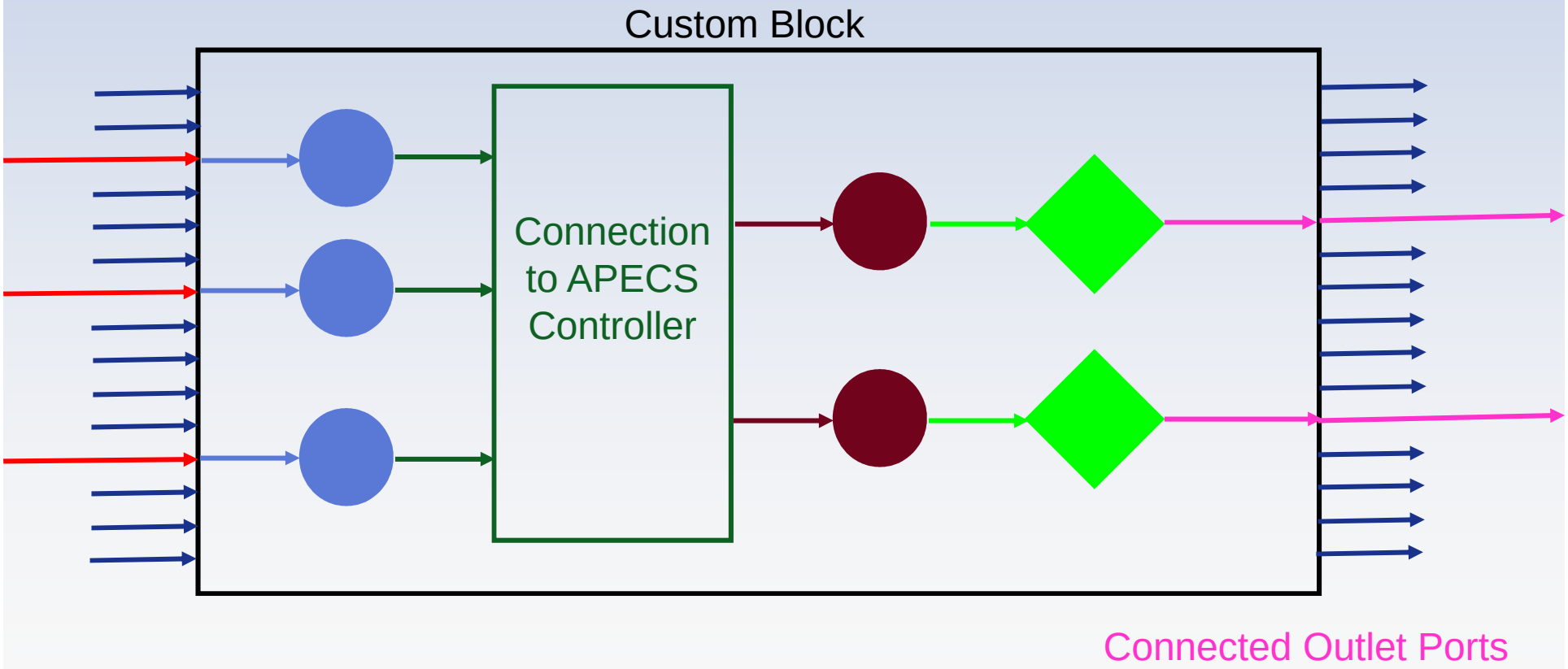
Aspen Dynamics Wrapper (cont.)

- **Custom block created in Aspen Custom Modeler**



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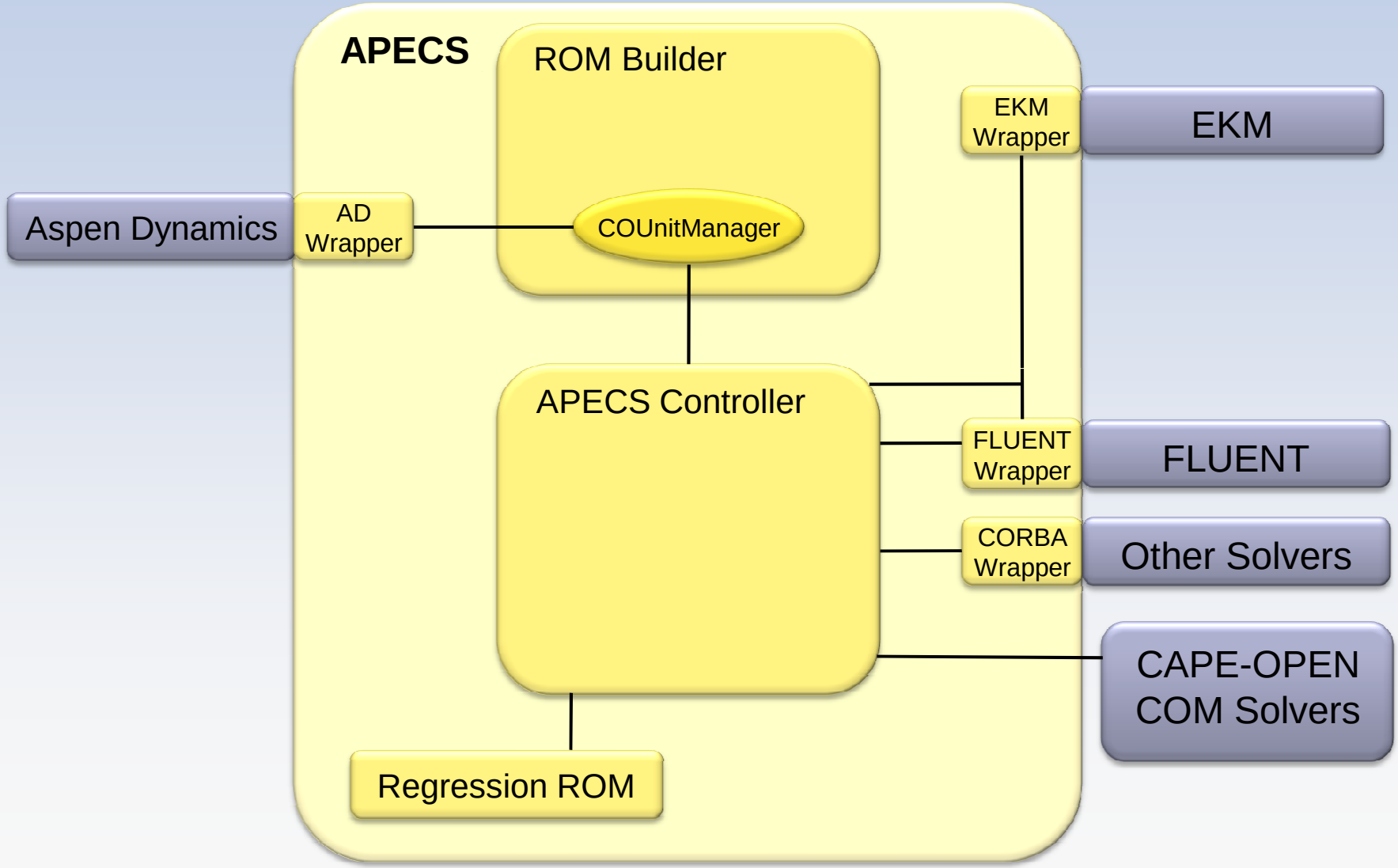
Architecture for Dynamic Co-Simulation



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Aspen Dynamics Wrapper Functions

	INITIAL APPROACH	FINAL APPROACH
PRECALL		Create COUnitManager Start FLUENT Load Case/Data files
OUTPUTS	Create COUnitManager Start FLUENT Load Case/Data files Set boundary conditions Converge FLUENT model Return outputs Exit FLUENT Clean up	Set boundary conditions Converge FLUENT model Return outputs
POSTCALL		Exit FLUENT Clean up

PRECALL ➡ OUTPUTS ➡ OUTPUTS ➡ … ➡ OUTPUTS ➡ POSTCALL

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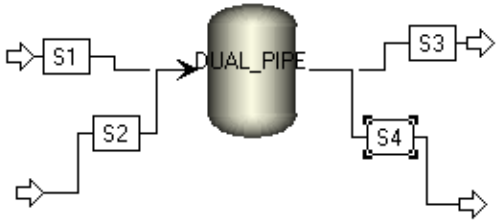
Test 1 – Verify Correct Outputs

- **2D FLUENT "Dual Pipe" model**
  - 2 inlets / 2 outlets, no mixing



S1.AllVariables Table

	Value	Spec	Units
<ComponentList	Default		
<Connected	TRUE		
<F	20.0	Fixed	kmol/hr
<h	500.0	Fixed	GJ/kmol
<P	1.0	Fixed	bar
<PortName	inlet_1		
<T	40.0	Fixed	C
<V	0.05	Fixed	m3/kmol
<z("ETOH")	0.2	Fixed	kmol/kmol
<z("H2O")	0.2	Fixed	kmol/kmol
<z("MEOH")	0.6	Fixed	kmol/kmol

S3.AllVariables Table

	Value	Spec	Units
>ComponentList	Default		
>Connected	TRUE		
>F	19.9825	Free	kmol/hr
>h	-0.25426	Free	GJ/kmol
>P	1.01325	Free	bar
>PortName	outlet_1		
>T	39.75	Free	C
>V	0.0402705	Free	m3/kmol
>z("ETOH")	0.199792	Free	kmol/kmol
>z("H2O")	0.200005	Free	kmol/kmol
>z("MEOH")	0.600203	Free	kmol/kmol

S2.AllVariables Table

	Value	Spec	Units
<ComponentList	Default		
<Connected	TRUE		
<F	15.0	Fixed	kmol/hr
<h	0.05	Fixed	GJ/kmol
<P	1.0	Fixed	bar
<PortName	inlet_2		
<T	30.0	Fixed	C
<V	0.05	Fixed	m3/kmol
<z("ETOH")	0.4	Fixed	kmol/kmol
<z("H2O")	0.4	Fixed	kmol/kmol
<z("MEOH")	0.2	Fixed	kmol/kmol

S4.AllVariables Table

	Value	Spec	Units
>ComponentList	Default		
>Connected	TRUE		
>F	15.0171	Free	kmol/hr
>h	-0.272453	Free	GJ/kmol
>P	1.01325	Free	bar
>PortName	outlet_2		
>T	30.25	Free	C
>V	0.0386318	Free	m3/kmol
>z("ETOH")	0.400055	Free	kmol/kmol
>z("H2O")	0.399737	Free	kmol/kmol
>z("MEOH")	0.200207	Free	kmol/kmol

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Test 2 – Benchmark Run Times

- **Case 1**
  - Pipe Model ROM Template
  - Fastest APECS block
  - Steady and Dynamic Co-Simulation
- **Case 2**
  - 2D FLUENT “Triple Pipe” model
  - 1200 quad cells
  - 3 inlets / 3 outlets, no mixing
  - Steady and Dynamic Co-Simulation

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Case 1 – Data Transferred

********** INPUTS **********

Block Name: PIPE_MODEL
Number of Inlet Ports: 10
Number of Outlet Ports: 10
Number of CONNECTED Inlet Ports: 1
Number of CONNECTED Outlet Ports: 1

Number of Species: 3
Specie 0 is ETOH
Specie 1 is H2O
Specie 2 is MEOH

Inlet Port Name = inlet_port
Inlet Flow Rate = 0.02 kg/s
Inlet Temperature = 313.15 K
Inlet Pressure = 100000.00 Pa
Inlet Mass Fraction [0] = 0.2876
Inlet Mass Fraction [1] = 0.1124
Inlet Mass Fraction [2] = 0.6000

Outlet Port Name = outlet_port

Persistence String 0 is InstanceKey_47
Persistence String 1 is UnusedPersistenceString_1
Persistence String 2 is UnusedPersistenceString_2

********** OUTPUTS **********

OUTPUTS was called 60 times
Retrieving the COUnitManager pointer. Block Name: PIPE_MODEL
Setting values of persistence strings in OUTPUTS now.

Persistence String 0 is now InstanceKey_47
Persistence String 1 is now UnusedPersistenceString_1
Persistence String 2 is now UnusedPersistenceString_2

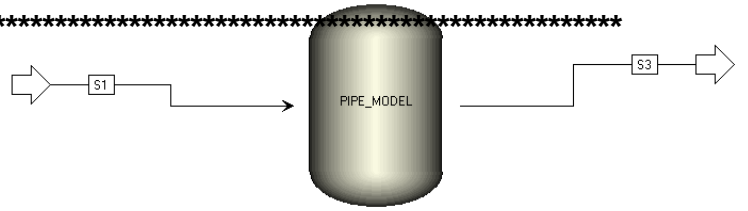
Outlet flow rate for outlet_port is 0.02 kg/s

Outlet temperature for outlet_port is 313.15 K

Outlet Pressure for outlet_port is 99000.00 Pa

Outlet Mass Fractions for outlet_port are:
Species [0]: 0.28755 (ETOH)
Species [1]: 0.11246 (H2O)
Species [2]: 0.59999 (MEOH)

****



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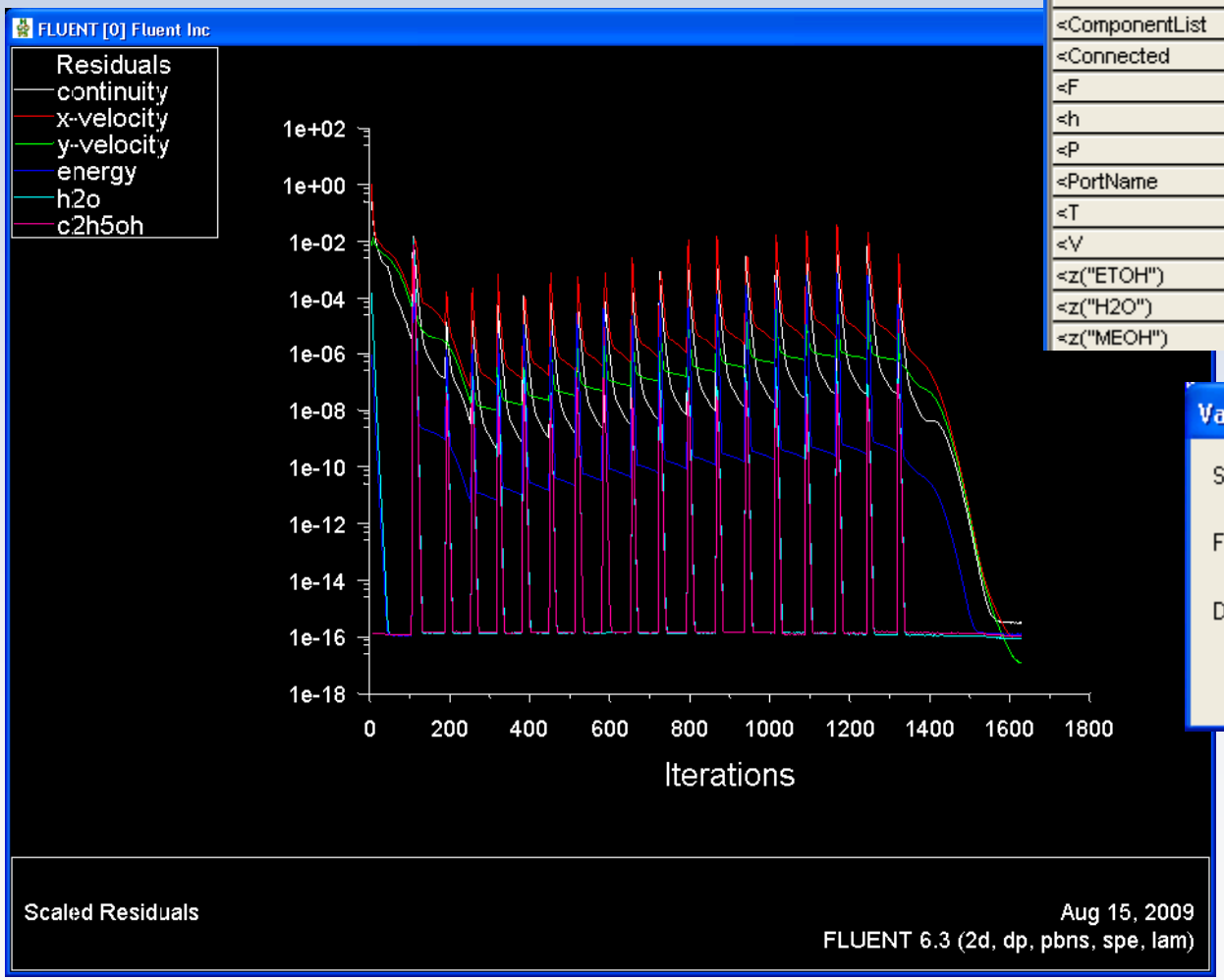
Case 2 – Dynamic Co-Simulation



S1.AllVariables Table

	Value	Spec
<ComponentList	Default	
<Connected	TRUE	
<F	10.0	Fixed
<h	500.0	Fixed
<P	1.0	Fixed
<PortName	inlet_1	
<T	80.0	Fixed
<V	0.05	Fixed
<z("ETOH")	0.2	Fixed
<z("H2O")	0.2	Fixed
<z("MEOH")	0.6	Fixed

Variable Ramp

Start time: 0 Seconds

Final value: 10 kmol/hr

Duration: 5 Seconds

OK Cancel

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Benchmark Results

Model	Mode	Inputs	Simulation Time, s	Real Time, s	"Output" Calls
Pipe Model ROM Template	Steady			407*	60
Pipe Model ROM Template	Unsteady	Steady	5	7200	1080
2D FLUENT Model	Steady			1096	60
2D FLUENT Model	Unsteady	Ramped (5 seconds)	10	22098	1380

*for comparison, this model takes ~1 second in Aspen Plus

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Summary

- **The feasibility of dynamic co-simulation was investigated**
- **A prototype Aspen Dynamics Wrapper was created to demonstrate dynamic co-simulation**
- **Run times were significantly longer for dynamic co-simulation than for steady co-simulation**
- **Promising future research: use ROMs capable of computing derivatives (e.g., Regression ROM) and return Jacobian to Aspen Dynamics**
  - Expected to significantly reduce the number of "Output" calls required

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